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Nitrocompounds: structure, force coefficients in coordinates X_{δ}^{0} and the frequencies of normal vibrations of NO_2-group

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Abstract

This article deals with geometric structure of number of *C*- and *N*-nitrocompounds. The matrix of the force coefficients in Cartesian coordinate system and in X_{δ}^{0} coordinates were calculated with the help of hybrid density functional theory (B3LYP/6-31(d,p)). The generalized force constants of couple vectors (X_{δ}^{0} coordinates) are presented here. The frequencies of normal vibrations of X-NO_2-fragment, where X = C,N were determine.